Supporting Information for

Coexistence of Open and Closed Type Nodal line Topological Semimetals in Two Dimensional B_2C

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I. PHONON BAND DISPERSION OF 2D FLATTEN B_2C.

We plot the phonon band dispersion of 2D flatten B_2C in figure S1. Clearly, negative frequency appear around high symmetry point Γ and along high symmetry line Γ-Y.

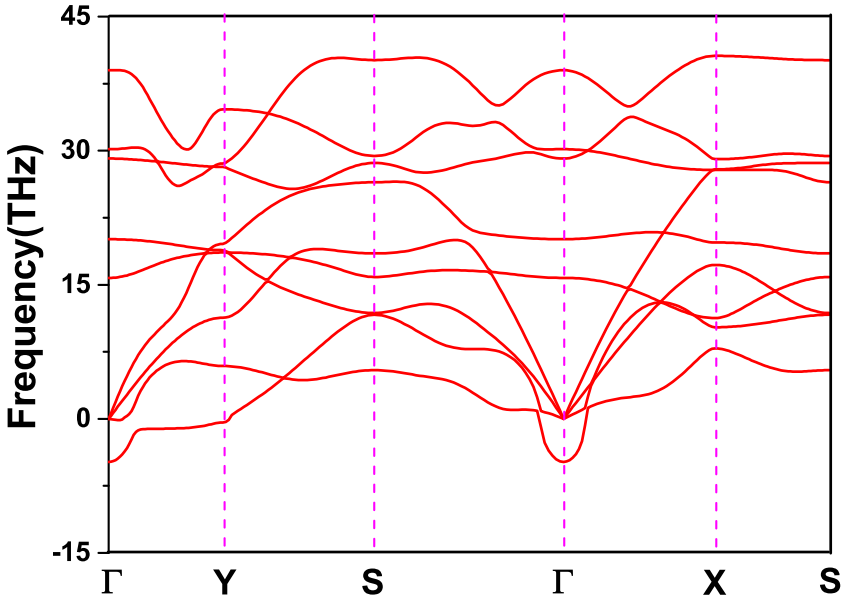

Figure S1: (color online) The Phonon band dispersion of 2D flatten B_2C.

II. THE ENERGY BAND STRUCTURE WITH HYBRID FUNCTION.

We further calculate the band structure with HSE06 hybrid functional calculations in structural relaxation and electronic self-consistent. Compared with the PBE's results. The crystal constant along x axis only reduced 0.57%(low buckled B_2C) and 0.69%(flatten B_2C). The y axis crystal constant almost no change. The results of energy band are shown in Fig.S2. (a) represent the result of low-buckled B_2C and (b) is flatten B_2C. The low energy band characters and the semimetal state discussed in our main manuscript are still exist in this exchange-correlation function. From the perspective of lattice symmetry, the semimetal states should exist because of hybrid functional wouldn't break the symmetry of 2D B_2C.

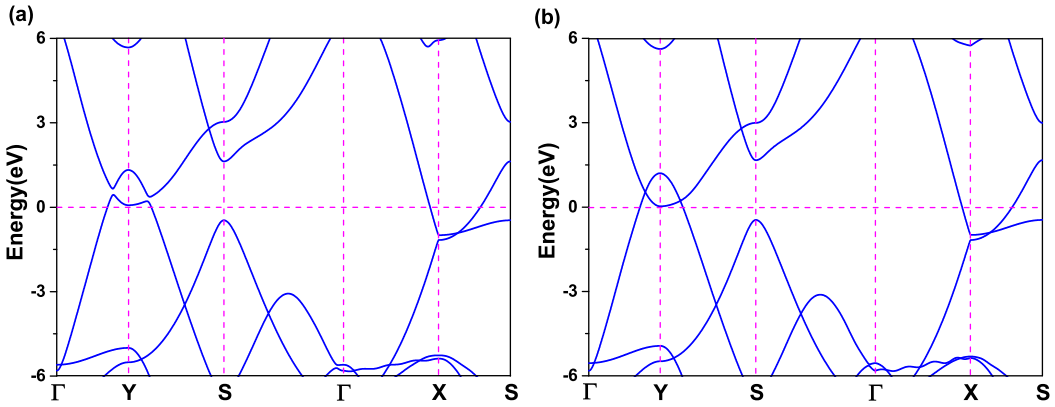

Figure S2: (color online) (a) Band structure of low-buckled B_2C with HSE06 hybrid function. (b) Band structure of flat B_2C with HSE06 hybrid function.

III. THE TIGHT BINDING PARAMETERS IN FIG.5(A)(B) OF MAIN MANUSCRIPTS

Table S1: The tight binding parameters in Fig.5(a)(b) of main manuscripts.

Parameters(eV)	ϵ_{1n}	ϵ_{2n}	ϵ_{3n}	t_{1n}	t_{2n}	t_{3n}	t_{4n}	t_{5n}	t_{6n}	t_{7n}
H_1(n=1)	-5.048	-13.554	-5.742	-1.434	-1.185	-0.543	-0.393	0.349	-0.266	-0.151
H_2(n=2)	-0.014	1.847	1.847	-2.367	-2.162	-1.477	0.443	0.519	0.283	

IV. THE STRUCTURE AND TOTAL ENERGY OF DIFFERENT B_2C CONFIGURES ON THE SURFACE OF CU(110)

With the help of CALYPSO code, we obtain many metastable structures of B_2C on the surface of Cu(110). Here we present some of structures and energy differences of them, as shown in figure S2. Comparing the configure in our main manuscript, a slight translation occurs for B_2C relative to the substrate in (a)(b)(c). Therefore, the energy difference of them are very small. The relatively higher energy of configure (d) and (e) indicate that other B_2C on the surface of Cu(110) or B atom embed into the groove of Cu(110) surface are very unstable.

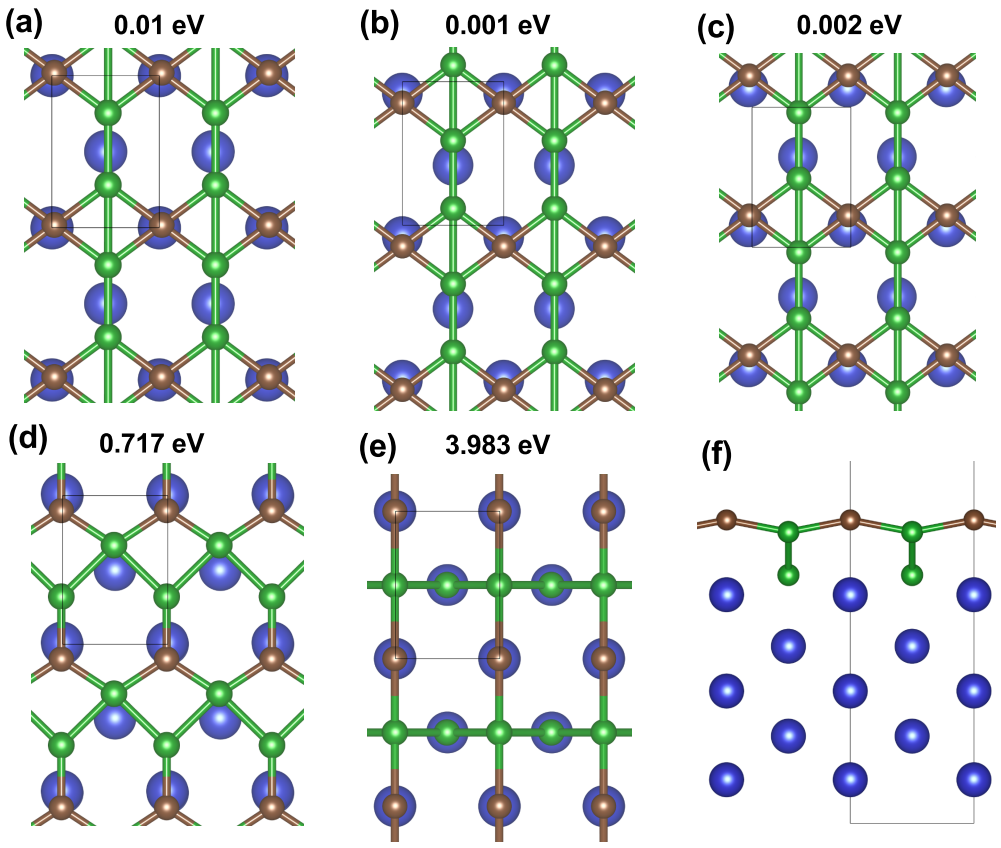

Figure S3: (color online) The structure and total energy of different B_2C configures on the surface of Cu(110). In the top view of (a)(b)(c)(d), the B and C atoms almost share the same 2D plane. (d) and (e) are the top view and side view of same configure.

V. THE STRUCTURE OF BILAYER B_2C SYNTHESIZED ON THE SURFACE OF CU(110) AND THE ENERGY BAND ALONG HIGH SYMMETRY LINES OF THE TOP LAYER B_2C.

Comparing with the van der Waals interaction, the interaction between monolayer B_2C and Cu substrate is stronger(2.12 Å). Therefore, the p_z of pristine B_2C are strongly affected by the Cu substrate. From the discussions in our main manuscript, we know that the p_z states of B and C atoms participate the formation of all semimetal states. In order to detect all semimetal in experiment, here we assume the first B_2C act as buffer layer, and another layer B_2C synthesized on the first layer with Van der Waals interactions(3.42 Å). The structure are depicted in Figure S3(a)(b). With the help of maximal localized Wannier function, we plot the energy band structure of the top layer B_2C, we found three types of semimetal states(type-I, type-II Dirac semimetals and open nodal line) are well kept. However, small band gap exist around the closed nodal line for flatten B_2C, which mean this nodal line is very sensitive to the weak interaction between B_2C and substrate. If we must observe the closed nodal line in B_2C, a kind of more inert buffer materials, for example 2D BN, should be placed between B_2C and metal substrate.

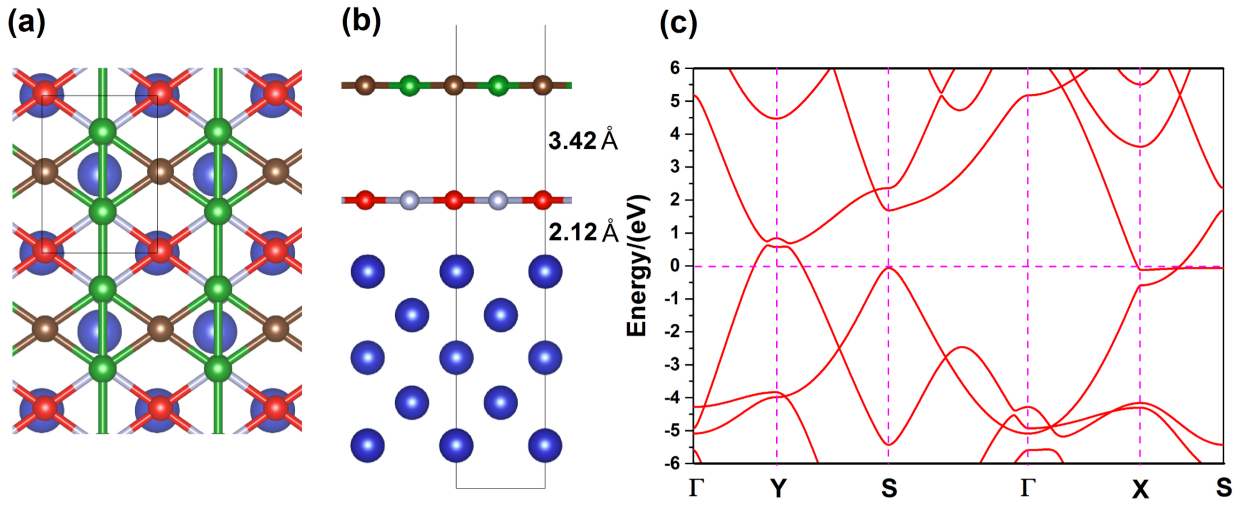

Figure S4: (color online) (a)(b) The top and side view of bilayer B_2C synthesized on the surface of Cu(110), we use the different color to label the first and the second layer B_2C. The red and black color represent C atoms, and the gray and green color are B atoms. (c) The energy band structure along high symmetry lines of the top layer B_2C.

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